

## ABSTRACT

The present invention provides a crystalline form of a substantially pure constitutive androstane receptor (CAR) polypeptide. Also provided is a crystalline form of a substantially pure constitutive androstane receptor (CAR) polypeptide in complex with a ligand. Also provided are methods for generating the crystalline forms of the present invention and methods for identifying and designing CAR ligands and modulators. Also provided are scalable three-dimensional configurations of points and computer readable storage media containing digitally encoded structural data.